Preparation, Crystal Structure and Thermodynamic Properties of $[Eu(NTO)_3(H_2O)_5]\cdot 5H_2O$

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Much attention has been paid to 3-nitro-1,2,4-triazol-5-one (NTO) as a high energy and low sensitivity energetic material. Its metal salts also have some potential uses in ammunition. Therefore the authors have prepared the single crystal of europium salt of NTO, measured its structure and studied its thermodynamic properties.

An appropriate amount of NTO is put into the distilled water (M:V = 1:4), then stirred and titrated with aqueous solution of lithium hydroxide under 60º until a pH at about about 7 is reached. The prepared solution is gradually dropped to the dilute nitric acid solution of europium oxide at 60º to get yellow precipitates. The precipitate is recrystallized with distilled water at room temperature to obtain the yellow single crystal for X-ray measurement.

Dimensions of the single crystal used for X-ray measurement are $0.15 \times 0.18 \times 0.22$ mm^3. X-ray intensities are recorded by a CAD4PDP 11/44 automatic diffractometer with graphite-monochromatized MoK_α radiation. 4692 independent reflections are obtained, among which 3896 with $I > 3.0\sigma(I)$ are used for the determination and refinement of crystal structure. Lorentz-polarization correction is applied and in addition to one for absorption correction. The crystalline structure is monoclinic, $P2_1/n$. The obtained crystallographic parameters are: a = 1.8720(2) nm, b = 0.6548(3) nm, c = 1.9323(3) nm, β = 95.33(1)°, V = 2.3583(5) nm^3, Z = 4, D_c = 2.026 g·cm^{-3}, μ = 27.678 cm^{-1}, F(000) = 1432. The final R is 0.0233.

From measurements of the enthalpy of solution in water of $[Eu(NTO)_3(H_2O)_5]\cdot 5H_2O$ at 298.15 K, the standard enthalpy of formation, lattice enthalpy, lattice energy and standard enthalpy of dehydration have been determined as – (3797.6 ± 6.8), – 4488, –4452, and 275.3 kJ·mol^{-1}, respectively.